1014-92-1734 **Victoria A Shimanovich***, 14 McLean Hall, Department of Mathematics, University of Iowa, Iowa City, IA 52242, and **Alberto Maria Segre**. *Comparison of Different Optimization Techniques Applied to the Soft Protein Docking Problem.*

Two proteins can interact only if their chemical properties permit and their geometric shapes allow them to, therefore, the protein docking problem, in its simpliest form, is essentially a mechanical problem of fit and subsequent match of binding areas. Modeling protein interactions involves two steps: finding the binding region, i.e., predicting a broad surface region of a protein whose shape may fit the shape of the other protein involved in the interaction, and then refining those sites into highly affine complex structures. In mathematical terms, this translates into a two-step optimization problem: finding a feasible region, and then finding a locally-optimal solution within the feasible region. In our work we allow certain sidechain and portions of backbone to exhibit a certain degree of flexibility. We focus on interactions within one protein since it models the same binding process as in protein-protein interaction, with the only difference being that the binding regions come from one macromolecule instead of two. In our problem we will use a hybrid approach combining a distributed search technique and a continuous optimization techniques. We compare different optimization methods to ensure the best results for the solution of the Soft Protein Docking Problem. (Received September 29, 2005)